ALASKA DEPARTMENT OF ENVIRONMENTAL CONSERVATION
DIVISION OF SPILL PREVENTION AND RESPONSE
CONTAMINATED SITES REMEDIATION PROGRAM

Guidance No. CSRP-98-001 July 6, 1998

GUIDANCE FOR FATE AND TRANSPORT MODELING

PURPOSE:

The attached guidance document is to provide general guidelines for the application of fate and transport models, including the planning and evaluation of models, and to promote the appropriate use of models.

BACKGROUND:

Fate and transport models have become an integral tool for contaminated site investigations and the selection of remedial techniques. Contaminated Sites Remediation Program (CSRP) uses contaminate fate and transport models as a tool for predicting contaminant concentrations at exposure points, and, to assist with the evaluation and selection of the most effective remedial alternative.

APPLICABILITY:

This guidance provides general guidelines to CSRP staff for the application of fate and transport models. This is not a substitute for professional judgment that must be applied in the selection and application of modeling.

DISCUSSION:

Contaminated Sites Remediation Program wants to ensure that modeling results are protective of human health and the environment. The effective use of predictive fate and transport models as management decision tools requires the establishment of their functionality, performance characteristics, and applicability to the site being considered.

ACTION:

Contaminated Sites Remediation Program suggests the use of this guidance while conducting fate and transport modeling at contaminated sites.

APPROVAL:

Lynn J. Tomich Kent

Lynn J. Tomich Kent
Program Manager

July 6, 1998
Date

G:\CSITES\POLICY\MOD_GIDC.WPD

Fate and Transport Modeling Guidance Contaminated Sites Remediation Program (CSRP) Alaska Department of Environmental Conservation

June 11, 1998

Introduction

Fate and transport models have become an integral tool for contaminated site investigations and the selection of remedial techniques nation-wide. The Alaska Department of Environmental Conservation, Contaminated Sites Remediation Program (CSRP) uses contaminate fate and transport models to help determine site specific aquifer characteristics, as a tool for predicting contaminant concentrations at exposure points; and to assist with the evaluation and selection of the most effective remedial alternative. CSRP recognizes that the use of fate and transport models will increase, and regulatory agencies will be relying on information obtained through modeling to assist with site management decisions.

CSRP project managers want to ensure that modeling results are protective of human health and the environment. At issue are the regulatory acceptance criteria for contaminant fate and transport models. The effective use of predictive fate and transport models as management decision tools requires the establishment of their functionality, performance characteristics, and applicability to the site being considered.

The purpose of this guidance is to provide general guidelines for the application of fate and transport models, including the planning and evaluation of models, and to promote the appropriate use of models. This guidance is not a substitute for professional judgment that must be applied in the selection and application of modeling. This guidance considers any predictive exercise that attempts to describe the future or the past movements of transporting media and/or contaminants as a model, either qualitative or quantitative, analytical or numerical.

Model selection requires site-specific evaluation

A list of models for use at all sites is not considered appropriate and therefore is not included with this guidance. The heterogeneous nature of transporting media, contaminant type and distribution, and, site-specific nature of projects require that models should be evaluated on a site-specific basis. Lists of fate and transport models, however, are available from many sources. For example, USEPA's Center for Subsurface Modeling Support[1] at Robert S. Kerr Environmental Research Center, and, U.S. Geological Survey[2]

[1] P.O. Box 1198, Ada, Oklahoma 74820. (405) 436-8500 http://www.epa.gov/ada/csmos.html

[2] http://water.usgs.gov/software/

maintain lists of models, downloadable softwares and manuals. The CSRP owns several modeling packages that are used as review tools. Consultants are encouraged to inquire as to the availability of a specific model within CSRP to ensure that CSRP project managers are familiar with and have access to a specific model.

Although CSRP does not maintain an approved list of models, the CSRP recommends that models with the following characteristics be selected for use:

1. The model should provide conservative predictions. With the uncertainty in model parameters and unknowns in subsurface (for example, a few fractures are always present in a porous medium) conservative prediction is critical.
2. The model should be technically sound and legally defensible
3. The model is within the public domain
4. Model information and reviews are published in reputable technical journals
5. The model has received adequate peer review.

Public Domain Modeling Programs

CSRP prefers that public domain computer programs be selected to assist with the remedial decision at a site for the following reasons:

1. ADEC project managers and term contractors are familiar with a number of public domain modeling programs.
2. ADEC project managers and term contractors normally do not have the time and resources to learn a unique computer modeling program for one specific project.
3. Proprietary modeling programs must be purchased by ADEC project managers and term contractors, thus adding to the overall cost of the project.
4. All ADEC projects, including modeling aspects of the project, are considered public information and must be available to the public for review.
5. By discouraging the use of proprietary models, it may seem that ADEC is suppressing creativity in model development. ADEC, however, is a government regulatory department, not a research organization. Review of numerical techniques used and computer source code are very time intensive. ADEC lacks adequate available resources to continuously evaluate new computer models. It is therefore unjustifiable for agency staff to review a modeling program every time a consultant submits a new one or modifies an old one.

For this guidance, “public domain modeling programs” are defined as readily available, widely distributed, and generally accepted models. The majority of the public domain models have received extensive peer-review, and case histories describing their limitations and drawbacks have been published in the scientific literature. Many of the public domain modeling programs were developed by government agencies, such as, USEPA, USGS and USDOD.

When a public domain program has been modified it can no longer be considered a public domain program. A modified public domain model can still be proposed for use if it is peer reviewed, widely distributed, and generally accepted. Compared to public domain modeling programs, proprietary modeling programs, without proper review and general acceptance, provide a lower level of confidence in making site cleanup decisions.

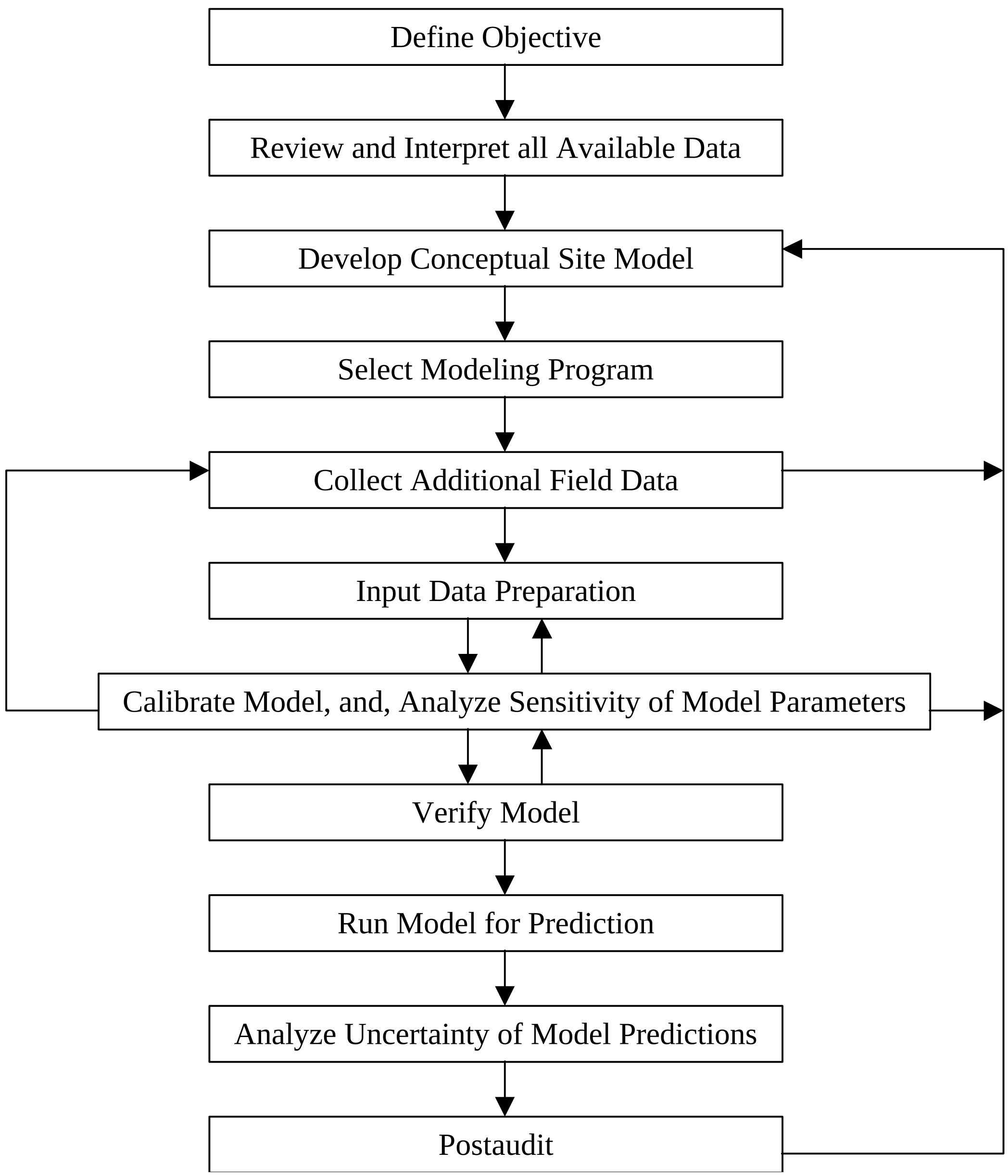

Figure 1: Steps in Contaminated Sites Model Application

Modeling Work Plan

Figure 1 outlines the steps involved in contaminated sites model application. A site investigation must precede modeling at a contaminated site. If a responsible party will use modeling, a modeling work plan must be submitted to CSRP for approval prior to use.

The modeling work plan may be a section of a work plan describing all proposed work at a contaminated site. The proposed modeling work plan should include the following components.

Modeling goals
The goals and reasons for the modeling should be specific and measurable. For example, modeling might be conducted in order to predict benzene concentrations in groundwater at a certain distance from a source of specified concentration, or, the prediction of vapor concentrations arising from a well-defined source in an enclosed space of specific dimensions. Having a specific goal helps determine, at a later time, if the modeling exercise has achieved the goal.

Conceptual Site Model for Modeling
Based on available data, regional inferences, and professional judgement, a geologic and hydrogeologic conceptual site model should be prepared and included in the work plan. The conceptual site model should be graphical (maps, cross-sections, block diagrams) with associated descriptions. If the conceptual site model will be simulating ground water flow, it must indicate whether subsurface is a porous or a fractured medium. The conceptual site model must quantify the presence of permafrost and corresponding influence on fluid flow. The conceptual site model must describe the temperature and pressure conditions of the transporting media. Finally, the conceptual site model should also discuss data gaps, assumptions, and uncertainties.

Technical Approach
Narrative should be included which describes technical considerations to achieve the stated goal, such as, numerical or analytical, modeling dimensions (1-D, 2-D or 3-D), saturated or unsaturated flow, multiphase or single phase, reactive or non-reactive, dispersion, retardation, and/or degradation.

Computer Model
The workplan should identify the computer model selected. Discussion of the abilities and limitations of the model in general, and, also in terms of the site-specific conceptual model should be included. Site-specific input parameters are preferred. The work plan should reference the specific reports where the data has previously been presented in addition to presenting the site-specific data, sample numbers, dates collected, and specific sample locations. Non site-specific input parameters should have good justifications. The source of these parameters should be identified, for example, USEPA's Soil Screening Guidance documents, ADEC Contaminated Sites' "Guidance on Cleanup Standards, Equations and Input Parameters" or scientific literature. The work plan should specify if input parameters have been assigned assumed values and justify the basis for the assumptions. The fate and transport parameters should be for the temperature and pressure conditions described in the conceptual model versus standard temperature and pressure conditions. Submit computations to derive the parameter values at site-specific temperature and pressure conditions from the standard temperature and pressure conditions. Boundary and

initial conditions should be described.

Sensitivity analysis
A plan to compute model sensitivity with the variation of calibrated input parameters within reasonable ranges to find more sensitive parameters.

Model calibration
A plan to calibrate the model to reproduce appropriate field-measured parameters. The field-measured parameters will be different for different models and for different transporting media. Calibration establishes that the model can reproduce field conditions. Models have no predictive value if they cannot reproduce observed concentrations.

Model verification
Plan to reproduce a second set of field data using the set of calibrated parameter values and stresses. Because of uncertainties in the calibration, parameter values of a calibrated model may not represent the contaminated site conditions. If the parameter values established during calibration are changed during verification, the model should be calibrated again with the changed parameter values. By reproducing a second set of field data, model verification establishes greater confidence in the model. With only one set of field data, it may not be possible to verify a model. A second set of field data collection is often possible at sites with multiple observation wells. CSRP may accept a calibrated but unverified model for predictions as long as careful sensitivity analysis of both the calibrated and the predictive models are performed and evaluated.

Uncertainty analysis
Describe the uncertainty associated with the modeling of a given problem. The uncertainty in modeling exists because uncertainties in transport mechanism, sink/source within the transporting media, temporal and spatial variation of model parameters, initial and boundary conditions, and, matrix heterogeneity.

Postaudit of modeling
Plan to conduct postaudit several years after the modeling study is completed. Collect new field data to determine whether the prediction was correct. Analyze what went wrong with modeling and means to improve it. If site remediation work reduces risks posed by the contaminated site to acceptable labels, and, monitoring proves that the risks are acceptable, a postaudit may not be necessary.

Modeling Report
A final modeling report should describe model predictions, technical analysis, input parameters, results of parameter sensitivity and model uncertainty analysis. Critical input and output files should be in the report's appendix, also in portable computer disks. The report should have sufficient information for an independent reviewer to duplicate model runs.

Model Review

CSRP may hire a term contractor to review the modeling work plan and modeling results. In accordance with State law, all expenses incurred for project oversight, including review of fate and transport models, must be reimbursed by the responsible party. If the modeling program is not available within CSRP, the consultant must provide a copy to the department, complying with any copyright laws. Model acceptance may require contaminant levels monitoring, and, institutional controls.

Annotated Bibliography

Alam, A. H. M. S. (1998, in preparation). “Regulatory Guidance on Fate and Transport Modeling.” 3rd International Conference (MODFLOW '98) on ground water modeling, organized by International Ground Water Modeling Center, U.S. Geological Survey, and, Waterways Experiment Stations of U.S. Army Corps of Engineers, October 4-8, 1998, in Golden, Colorado.

Alaska-specific issues are discussed in this paper. Regulators want to be certain that human health and the environment are being protected based on modeling results. The models must be legally defensible, technically sound, and must survive public scrutiny. Many contaminated sites are legally disputed, and a modeler should be able to defend technical basis, parameter values, and results of a model in a courtroom. A technically sound model has probably stood the test of time, underwent peer-reviews, and is widely accepted in scientific community. Affected public should be able to comprehend and concur with the model in their terms.

Anderson, M. D. and W. W. Woessner (1992). Applied Ground Water Modeling: Simulation of Flow and Advective Transport. San Diego, CA, Academic Press Inc.

An excellent text book on contaminant groundwater modeling. It discusses many topics related to MODFLOW, including discussing the steps involved in developing a groundwater model.

ASTM (American Society for Testing and Materials) (1996). ASTM Standards on Analysis of Hydrologic Parameters and Ground Water Modeling.

Compilation of ASTM standards on two specialized topics in one volume: determining aquifer properties and ground-water modeling.

ASTM (American Society for Testing and Materials) (1996). Subsurface Fluid-Flow (Ground-Water and Vadose Zone) Modeling.

Features techniques and guidance for simulating water, air and contaminant movement in subsurface water resources. Papers are presented in an order consistent with the procedures for conducting a model application. A comprehensive glossary of ground-water modeling terminology is included.

Bear, J., M. S. Beljin, and, R. R. Ross (1992). USEPA Groundwater Issue Paper -

Fundamentals of Ground-Water Modeling.
This paper presents an overview of the essential components of ground-water flow and contaminant transport modeling in saturated porous media.

Dougherty, D. E. and A. C. Bagtzoglou (1993). “A Caution on the Regulatory Use of Numerical Solute Transport Models.” Ground Water **31**(6): 1007-1010.
Numerical models of solute transport in water-saturated porous media are routinely used to make regulatory and design decisions. For many contaminants, decisions are based on concentrations of 5 parts per billion (ppb) or less. This "action level" is usually a small fraction (<0.01) of the concentrations near a source of contamination. Two one-dimensional example problems are used to demonstrate that modeling errors using classical numerical methods are largest where concentrations are lowest. This implies that in regions of low dimensionless concentration, that is near the action level, large relative errors can be expected. Hence, decisions based on numerical model solutions at low concentrations must be taken cautiously. Modern numerical methods for the solution of transport equations provide better behavior, in this sense, than classical methods.

Harr, J. (1995). A Civil Action, Random House, Inc.
Describes an environmental litigation for a contaminated site in Woburn, Massachusetts. Modelers representing both sides of the litigation testified to establish who was responsible for cleanup.

Kresic, N. (1997). Quantitative Solutions in Hydrogeology and Groundwater Modeling, Lewis Publishers.
Combines two disciplines - hydrogeology and groundwater modeling - and covers both theory and practice. This book addresses and solves a variety of questions and problems, and includes major aspects of quantitative groundwater evaluation, from basic laboratory determination of hydrogeological parameters to complex analytical calculations and modeling.

Lukas, I. (1997). “A Tiered Approach to Regulators' Evaluation of Groundwater Model Applications.” Remediation Management, First Quarter: 22-29.
Groundwater model applications could more effectively be used in regulatory decisionmaking if their evaluation was based on methods commonly agreed upon by the regulators and the regulated community.

Schmelling, S. G. and R. R. Ross (1989). EPA Superfund Ground Water Issue - Contaminant Transport in Fractured Media: Models for Decision Makers, U.S. EPA.
This paper summarizes the status of modeling ground-water flow and contaminant transport in fractured rock systems.

Spitz, K. and J. Moreno (1996). A Practical Guide to Groundwater and Solute Transport Modeling, Wiley Interscience.

> This book covers all three areas: model input data, the calibration of a model, and the development of model summaries. Compiled tables of typical hydraulic parameters, octanol-water partitioning coefficients, radioactive decay half-lives, and many other fate and transport parameters. Appendix A provides a concise overview of the steps involved in a groundwater modeling study.

U.S. EPA (1994). Assessment Framework for Ground-water Model Applications.

> This Assessment Framework addresses the use and review of primarily ground-water flow and advective transport model applications. The criteria in this Assessment Framework focus upon the activities and thought processes that should be part of a model application and the subsequent documentation of that activity or process.

U.S. EPA (1994). Environmental Services Division Guidelines - Hydrogeologic Modeling. Region 10, Seattle.

> The guidelines provide a list of elements to consider when conducting ground water and surface water flow, contaminant mass transport, and geochemical modeling.

U.S. EPA (1994). Ground-water Modeling Compendium - second edition, Model Factsheets, Descriptions, Applications and Cost Guidelines.

> The use of this Compendium is intended to help promote the appropriate use of models thus effecting sound and defensible modeling. It describes eight widely-used ground-water models. It provides summary descriptions of six model applications that illustrate the complexities of the use of models.

U.S. EPA (1996). Soil Screening Guidance: Technical Background Document, Office of Solid Waste and Emergency Response, Washington, D.C.

> The Soil Screening Guidance is a tool developed to help standardize and accelerate the evaluation and cleanup of contaminated soils at sites on the National Priorities List (NPL) where future residential land use is anticipated. The Technical Background Document presents the analysis and modeling upon which this approach is based, as well as generic SSLs calculated using conservative default values, and guidance for conducting more detailed analysis of complex site conditions, where needed.

U.S. EPA (1996). Soil Screening Guidance: User's Guide. Office of Solid Waste and Emergency Response, Washington, D.C.

> The Soil Screening Guidance is a tool developed to help standardize and accelerate the evaluation and cleanup of contaminated soils at sites on the

National Priorities List (NPL) where future residential land use is anticipated. The User's Guide provides a simple step-by-step methodology for environmental science/engineering professionals to calculate risk-based, site-specific soil screening levels (SSLs) for contaminants in soil that may be used to identify areas needing further investigation at NPL sites.

van der Heijde, P. K. M., A. I. El-Kadi, et al. (1989). Groundwater Modeling: An Overview and Status Report.

This report focuses on groundwater models and their application in the management of water resource systems. The report begins with the introduction of system concepts applicable to subsurface hydrology and presents groundwater modeling terminology, followed by a discussion of the role of modeling in groundwater management.

van der Heijde, P. K. M. and O. A. Elnawawy (1992). Quality Assurance and Quality Control in the Development and Application of Ground-water Models.

This report provides background information on quality assurance and defines the role of quality assurance and quality control in ground-water modeling. A functional and practical quality-assurance methodology is presented which is written from the perspective of the model user and the decision-maker in need of technical information on which to base technical decisions. An important part of quality assurance is code testing and performance evaluation. A section is included on code testing and performance evaluation presenting the three-level testing procedure developed by the International Ground Water Modeling Center, the development of test problems and related benchmarks for the first two test levels, and a discussion of the implementation of the testing procedure.

Zheng, C. and G. D. Bennett (1995). Applied Contaminant Transport Modeling-Theory and Practice, Van Nostrand Reinhold Publishers.

This book discusses the current research issues, but it deals primarily with practical aspects of transport modeling. The book is intended to serve as a reference for self-study or as an advanced textbook for college courses. The two parts of the book, concepts and field applications, represent the natural division of the topic.